ON THE THEORY OF NON-EQUILIBRIUM STATISTICAL PROCESSES

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A stochastic equation is derived by means of the phenomenological equations of motion under well-defined assumptions. The thermal noise of a nonlinear resistance is considered as an example.

IN view of the fact that a mathematical analysis of the exact dynamical picture of non-equilibrium statistical processes is very difficult, it is advisable to study such processes using equations of the phenomenological type. This leaves only a small number of coordinates to be considered (the coordinates of a Brownian particle, the charge or current in an electrical circuit, and so on). The participation of a huge number of other particles in the process expresses itself implicitly in two ways. Firstly, there is dissipation, which is described by the phenomenological equation for the average velocity-dependent force (elementary dynamical interactions are non-dissipative). Secondly, there are the fluctuating impacts from the surrounding medium. The average phenomenological force defines the first-derivative term in the stochastic equation, while the fluctuating impacts cause the occurrence of terms (or a term) with higher derivatives. An evaluation of the statistics of the fluctuating actions so as to determine the form of these terms is a more difficult problem than the determination of the average phenomenological force. The latter can be determined experimentally and can be considered as given in the theory. From general considerations it follows that there is a connection between the statistics of the fluctuating actions and the dissipation in the system. The determination of these statistics from the dissipation mechanism is a general and important problem in statistical physics and has many diverse applications.

For the case where the dissipative force depends linearly on the velocity the above problem was solved in the classical papers on Brownian motion (Langevin and others). The problem is, however, appreciably more complicated in the case of a nonlinear mechanism of dissipation, and has not yet been solved in general form at the present. Some authors (see, for instance, reference 1) even deny the existence of a necessarily unique connection between the average force and the intensity of the impacts in the general case. The papers of Magalinskiĭ and Terletskiĭ[2-4] were devoted to a consideration of the above mentioned problem, but gave rise to important objections.

In the present paper we give an exact solution of a well-defined problem; that is to say, we derive a stochastic equation under the assumption that the relaxation time for the velocity is much smaller than the relaxation time for the coordinate. To do this we apply a method based on a corrected and extended version of the method proposed in references 2 — 4.

Let q be one or several coordinates of an arbitrary mechanical system described by a Hamiltonian $H(p, p', q, q')$ (the q' are the remaining coordinates). The process of motion is determined by the dynamical equations

$$\dot{q} = \partial H / \partial p, \qquad \dot{p} = -\partial H / \partial q. \tag{1}$$

The totality of the influence of the variables q', which correspond to the medium through which the particle moves, can be described phenomenologically by introducing a frictional force (in the general case nonlinear) and fluctuating forces. The exact Eqs. (1) are then replaced by a phenomenological equation of the Langevin type

$$\ddot{q} = \Phi(\dot{q}, q, t) = F(\dot{q}, q) + \xi(t, \dot{q}, q). \tag{2}$$

We assume that the kinetic energy pertaining to the coordinate q is equal to $m\dot{q}^2/2$. The function Φ in (2) has the meaning of a force divided by the mass m. The division by m was performed to simplify the formulae and we shall continue to call Φ a "force."

The force Φ is given in (2) as the sum of an average force, $F = \overline{\Phi}$, and a fluctuating term which by definition has an average value of zero:

$$\overline{\xi(t,\ q,\ q)} = 0. \tag{3}$$

For the sake of simplicity, we have chosen to write our equations in one-dimensional form (q is one coordinate).

The dependence of the force on the coordinate and on the velocity can be determined experimentally. One must average the action of the fluctuating force in that case over some time interval τ_y, which must be longer than the correlation time τ_1 of the fluctuating force: $\tau_y \gg \tau_1$. The length of the time interval over which it is averaged has no upper bound. However, to obtain as detailed a phenomenological description of the system as possible, it is desirable to choose the smallest value compatible with the above-mentioned inequality.

What we can measure is essentially not the exact force Φ as a function of q and $\dot{q}$, but an average force $\tilde{\Phi}$ as a function of the average values q and $\tilde{\dot{q}}$. The tilde on top indicates here an average over the time τ_y, for instance,

$$\tilde{\dot{q}} = \frac{1}{\tau_y}\int_t^{t+\tau_y} \dot{q}\,dt = \frac{q(t+\tau_y)-q(t)}{\tau_y}. \tag{4}$$

Because of the condition $\tau_y \gg \tau_1$ $\tilde{\Phi}$ is the same as F. If we wish to find out how $\tilde{q}$ and $\tilde{\dot{q}}$ are connected with the instantaneous values q and $\dot{q}$, we must take into account the relaxation times of the latter. We introduced along with τ_1 the velocity relaxation time

$$\tau_2 \sim \tilde{\dot{q}}/\tilde{\ddot{q}} \sim \tilde{\dot{q}}/F \tag{5}$$

and the coordinate relaxation time

$$\tau_3 \sim \tilde{q}/\tilde{\dot{q}}. \tag{6}$$

Different relations are possible between the time constants τ_1, τ_2, and τ_3. We consider the case where

$$\tau_2 \ll \tau_3 \tag{7}$$

and where we can consider phenomenological equations that correspond to a time of averaging which satisfies the inequalities

$$\tau_y \ll \tau_3, \tag{8}$$

$$\tau_y \gg \tau_2. \tag{9}$$

Assume, in particular, that (7) is satisfied and the force relaxation time τ_1 is comparable with τ_2

$$\tau_1 \sim \tau_2. \tag{10}$$

If we then choose our averaging time so that $\tau_1 \ll \tau_y \ll \tau_3$, we satisfy conditions (8) and (9).

Because of inequality (8), $\tilde{q}$ is the same as q but $\tilde{\dot{q}}$ differs from the instantaneous value of $\dot{q}$. The trajectory in phase space is no longer a Markov process. Because of (7) the $q(t)$ process can, however, be considered to be a Markov process. Our problem is to express its statistical characteristics through the experimental function $F(\tilde{\dot{q}}, q)$, which is supposed to be known.

Inequality (9) enables us to state that the time average is the same as the statistical average

$$\tilde{\dot{q}} = \bar{\dot{q}} \tag{11}$$

[we are considering an ensemble for which $q(t_0) = q_0$]. This average value is independent of the initial velocity $\dot{q}(t_0)$, the influence of which vanishes within a period of time of the order of τ_2. It is thus some phenomenological function of the coordinate,

$$\bar{\dot{q}} = f(q). \tag{12}$$

Taking (11) into account we can write the phenomenological equation (2) in the form

$$\dot{v} = F(\bar{v},\ q) + \xi(t,\ \bar{v},\ q) \quad (v = \dot{q}). \tag{13}$$

The function (12) can be determined from Eq. (13). Indeed, averaging (13) and taking (3) into account, we find

$$\bar{\dot{v}} = F(\bar{v},\ p).$$

Substituting (12) and performing the transformation

$$\bar{\dot{v}} = \overline{\dot{f}(q)} = (\partial f/\partial q)\,\bar{v},$$

we obtain the equation

$$\partial f/\partial q = F(f,\ q)/f, \tag{14}$$

from which we can determine $f(q)$. One can simplify this with the aid of (7). To do this we take into account Eqs. (5) and (6) which define τ_2 and τ_3. The latter can be written

$$\tau_3^{-1} \sim f/q \sim \partial f/\partial q. \tag{15}$$

According to (5) $F/\bar{v}$ is of the order of $1/\tau_2$ for most values of $\bar{v}$; in our case, however, it is of order $1/\tau_3$, [i.e., appreciably smaller, because of (7)] as can be seen from (14) and (15). This exceptional value must be determined from the equation

$$F(\bar{v},\ q) = 0. \tag{16}$$

The latter states that an average velocity is set up in such a way that it corresponds to a zero force acting upon the particle.

Turning to the dynamical equations (1), we shall consider instead of the variables q and p the coordinate and velocity q and $v = \dot{q}$. In that case Eq. (1) is transformed into

$$\dot{q} = v, \quad \dot{v} = G(q, v, p', q') = -m^{-1}\partial H/\partial q. \tag{17}$$

Here $G(q, v, p', q')$ is the dynamical expression for the force, corresponding to the phenomenological expression Φ. The probability distribution density $w = w(q, v, p', q')$ changes according to the equation

$$\dot{w} = -\frac{\partial}{\partial q}(vw) - \frac{\partial}{\partial v}(Gw) + \frac{\partial H}{\partial q'}\frac{\partial w}{\partial p'} - \frac{\partial H}{\partial p'}\frac{\partial w}{\partial p'} \equiv Aw. \tag{18}$$

We are especially interested in the well-defined initial condition $q = q_0$ at $t = t_0$, which corresponds to

$$[w]_{t=t_0} = \delta(q - q_0)\, w_0(v, p', q') \tag{19}$$

(the initial distribution $w_0(v, p', q')$ does not play a large part since it relaxes rapidly).

We introduce the functions

$$W = e^{uq}w, \tag{20}$$

$$Z(u) = \int W d\Omega = \int e^{uq} w d\Omega, \tag{21}$$

$$\tilde{w} = W/Z(u) \tag{22}$$

($d\Omega = dq\, dv\, dp'\, dq'$) and ascertain their time variation. Writing (18) in the form

$$e^{-uq}\dot{W} = A(e^{-uq}W)$$

and differentiating we get

$$\dot{W} = AW + uvW. \tag{23}$$

If we integrate this equation over v and q we get

$$\dot{Z}(u) = u\bar{v}W, \tag{24}$$

where

$$\bar{v} = Z^{-1}\int vW d\Omega = \int v\tilde{w} d\Omega. \tag{25}$$

Differentiating $\tilde{w}$ with respect to time and substituting (23) and (24), we find

$$\dot{\tilde{w}} = A\tilde{w} + u(v - \bar{v})\tilde{w}. \tag{26}$$

We write the last term in (26) as a differential expression

$$(v - \bar{v})\tilde{w} = \sum_{m,\, n=0}^{\infty} \frac{1}{m!\, n!}\left(-\frac{\partial}{\partial q}\right)^m \left(-\frac{\partial}{\partial v}\right)^n (\beta_{mn}\tilde{w}). \tag{27}$$

Here $\beta_{mn} = \beta_{mn}(q_0)$ are suitably chosen coefficients. It is shown in the Appendix that they can easily be expressed in terms of the correlation functions of the velocity fluctuations; in particular,

$$\beta_{01} = \overline{(v - \bar{v})^2} = k_2(0),$$

$$\beta_{10} = \overline{(q - \bar{q})(v - \bar{v})} = \int_0^\infty k_2(\tau)\, d\tau. \tag{28}$$

Because of (27), Eq. (26) is equivalent to

$$\dot{q} = v + a(t), \quad \dot{v} = G(q, v, p', q') + b(t), \tag{29}$$

where $a(t)$ and $b(t)$ are random functions with average values

$$\bar{a} = u\beta_{10}, \quad \bar{b} = u\beta_{01}, \tag{30}$$

and with correlation functions (for r quantities a and s quantities b)

$$k_{(r)a,\,(s)b}(t_1, \ldots, t_{r+s}, q_0)$$
$$= u\beta_{rs}\delta(t_2 - t_1) \ldots \delta(t_{r+s} - t_1) \tag{31}$$

(cf. reference 5).

Equations (29) enable us to interpret $\tilde{w}$ as the distribution density for some new mechanical system subjected to additional forces a and b, each with a steady and a fluctuating term.

The additional forces can be included not only in the dynamic, but also in the phenomenological equations. In accordance with (29), Eqs. (13) are replaced by

$$\dot{q} = v + a(t), \quad \dot{v} = F(\bar{v}, q) + \xi(t) + b(t), \tag{32}$$

We use (32) to find a new phenomenological function

$$\bar{\dot{q}} = f(q, u), \tag{33}$$

which determines the average velocity. Averaging (32), we have

$$\bar{\dot{q}} = \bar{v} + \bar{a}, \quad \bar{\dot{v}} = F(\bar{v}, q) + \bar{b}. \tag{34}$$

As in the derivation of Eq. (16), we find from the second equation of (34)

$$F(\bar{v}, q) + \bar{b} = 0. \tag{35}$$

Solving with respect to $\bar{v}$ and denoting the corresponding function by f_1, we get

$$\bar{v} = f_1(q, u). \tag{36}$$

Substituting (36) into the first equation of (34), we get the required function (33):

$$\bar{\dot{q}} = f(q, u) = f_1(q, u) + \bar{a}. \tag{37}$$

The function (12) is, of course, none other than a particular value, $f(q, 0)$.

We now turn to the problem of the diffusion of an initial distribution of the type (19). In the first period, while $t - t_0 \lesssim \tau_2$, the fluctuations of $q(t)$ are not like a Markov process. Thereafter, when $\tau_2 \ll t - t_0 \ll \tau_3$ the average velocity $\bar{\dot{q}}$ approaches the function (12), which is independent of the initial velocity. For those intervals of time, the fluctuating process $q(t)$ can at the same time be considered to be a Markov process. The distribution $w(q, q_0)$, obtained from the initial distribution $\delta(q - q_0)$, then generates a Markov transition probability and characterizes completely the fluctuating process. For time intervals satisfying the condition

$$\tau_2 \ll t - t_0 \ll \tau_3,$$

the coordinate q does not have time to change strongly, and we have from Eq. (33), for the chosen initial condition,

$$\bar{q} = q_0 + (t - t_0) f(q_0, u). \tag{38}$$

According to what has been said above, the averaging $\bar{q}$ is then done over an ensemble corresponding to the included additional forces a, b, i.e., with the weight of w. According to (20) -- (22), this average can be written as

$$\bar{q} = \int q\tilde{w} d\Omega = \frac{1}{Z} \int q e^{uq} w d\Omega = \frac{1}{Z} \frac{\partial Z}{\partial u}. \tag{39}$$

Because of this (38) goes over into the equation

$$\partial \ln Z(u)/\partial u = q_0 + (t - t_0) f(q_0, u), \tag{40}$$

from which we can determine Z(u). When integrating this we take into account the initial condition Z(0) = 1, which follows from (21), and we get

$$Z(u) = \exp\{q_0 u + (t - t_0) \int_0^u f(q_0, u)\, du\}. \tag{41}$$

For imaginary values of the argument u = iv the function Z(u) is none other than the characteristic function $\overline{\exp(iv)}$. The required transition probability can thus be obtained from it by a Fourier transformation

$$w(q, q_0) = \frac{1}{2\pi} \int e^{-ivq} Z(iv)\, dv. \tag{42}$$

Knowing the transition probability one can evaluate how any other initial distribution $w(q_0, t_0)$ will change. The Markov condition leads to

$$w(q, t) = \int w(q, q_0)\, w(q_0, t_0)\, dq_0. \tag{43}$$

The choice of the initial moment is arbitrary; giving t_0 increasing values we can follow the complete evolution of the distribution density.

It is convenient to consider a differential stochastic equation. To get it we expand (40) in powers of $t - t_0$. Retaining only the first two terms we have

$$Z(u) = e^{q_0 u} + (t - t_0) e^{q_0 u} \sum_{s=1}^{\infty} \frac{u^s}{s!} K_s(q_0). \tag{44}$$

The function $\int_0^u f(q_0, u)\, du$ is here expanded in a Maclaurin series and

$$K_s(q_0) = [\partial^{s-1} f(q_0, u)/\partial u^{s-1}]_{u=0}. \tag{45}$$

After substituting (44) into (42) we find

$$w(q, q_0) = \delta(q - q_0) + (t - t_0) \sum_{s=1}^{\infty} \frac{1}{s!} \left(-\frac{\partial}{\partial q}\right)^s K_s(q_0)\, \delta(q - q_0). \tag{46}$$

To obtain the stochastic equation we must still substitute (46) into (43). The term $w(q, t_0)$ obtained after integrating with $\delta(q - q_0)$ is shifted to the left-hand side and $[w(q, t) - w(q, t_0)]/(t - t_0)$ is denoted $\dot{w}$. The result is

$$\dot{w}(q) = \sum_{s=1}^{\infty} \frac{1}{s!} (-1)^s \frac{\partial^s}{\partial q^s} [K_s(q)\, w(q)]. \tag{47}$$

From a mathematical point of view, the main result here is that the correlation functions [or, what is the same, the moments $\overline{\eta(t_1, q) \ldots \eta(t_s, q)}$] of the random functions $\eta(t, q)$ in the equation

$$\dot{q} = f(q) + \eta(t, q), \tag{48}$$

which is equivalent to (47), cannot be given arbitrarily, but are uniquely determined by the force function F(q, v).

First example. A particle experiencing nonlinear friction. Let a conservative force g(q) and a nonlinear frictional force $\varphi(v)$ act upon the particle. The phenomenological Eq. (13) is of the form

$$m\dot{v} = g(q) - \varphi(v) + m\xi, \qquad \dot{q} = v. \tag{49}$$

In this case

$$\tau_2 \sim m/\varphi', \qquad \tau_3 \sim q\varphi'/g.$$

The condition for the applicability of the theory given here is thus of the form

$$m/\varphi' \ll \tau_y \ll q\varphi'/g. \tag{50}$$

The system with the additional forces included is described by the phenomenological equations

$$\dot{q} = v + a, \qquad m\dot{v} = g(q) - \varphi(\bar{v}) + m\xi + mb.$$

Averaging these and solving the equation

$$\varphi(\bar{v}) = g(q) + m\bar{b},$$

which corresponds to Eq. (35), we find

$$\bar{\dot{q}} = \bar{a} + \psi(m\bar{b} + g).$$

Here ψ is the inverse of $\varphi(v)$. According to (28) and (30) we then have

$$\bar{a} = u\beta_{10} = u\overline{(q - \bar{q})(v - \bar{v})}, \qquad \bar{b} = u\beta_{01} = u\overline{(v - \bar{v})^2}.$$

In view of the fact that the velocity distribution at time $t - t_0 \gg \tau_2$ is practically the same as at equilibrium, i.e., a Maxwell distribution, we have $m\bar{b} = u\Theta$ (Θ is the temperature).

The coefficients in (47) are evaluated from the equations

$$f(q, u) = u\beta_{10} + \psi(u\Theta + g); \qquad K_1 = \psi(g),$$

$$K_2 = \beta_{10} + \Theta\psi'(g), \quad K_n = \Theta^{n-1}\psi^{(n-1)}(g) \quad (n = 3, 4, \ldots). \tag{51}$$

To evaluate β_{10} it is expedient to take into account that

$$\overline{(q-\bar{q})(v-\bar{v})} = \tfrac{1}{2}\, d\,\overline{(q-\bar{q})^2}/dt = \tfrac{1}{2}\, d(K_2 t)/dt$$

and, thus, $\beta_{10} = \frac{1}{2}K_2$.

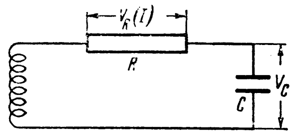
Taking (37) and (45) into account we get

$$K_2 = 2\Theta\psi'(g) = 2\Theta/\varphi'(K_1). \tag{52}$$

In the particular case where the frictional function is linear $[\varphi(v) = \beta v]$ the relation given here gives the usual expressions

$$K_1 = g/\beta, \qquad K_2 = 2\Theta/\beta, \qquad K_3 = \cdots = 0.$$

Second example. The mechanical example considered is analogous to an electrical circuit containing a nonlinear resistance and a nonlinear capacitance (Figure). q is then the charge on the capaci-



tance and $\dot{q} = I$ the current in the circuit, while the induction L plays the role of the mass. The relaxation times are in this case equal to

$$\tau_2 \sim L/R, \qquad \tau_3 \sim RC$$

$[R = dV_R/dI,\ C = V_C/q = g(q)/q]$. We can use for this circuit Eq. (46) with the values of the coefficients from (51), if

$$L/\bar{R} \ll RC \tag{53}$$

and if $\varphi(I)$ is taken to mean the function that describes the dependence of the average potential across the resistance on the average current after a time $\tau_y \gg L/R$

$$V_R = \varphi(\bar{I}).$$

When the dependence of the voltage on the instantaneous current

$$V_R = V(I)$$

(which corresponds to $\tau_1 \ll \tau_y \ll \tau_2$) is known from experiments, we can find the function φ corresponding to longer averaging times from the formula

$$\varphi(\bar{I}) = \sqrt{L/2\pi\Theta}\int V(I)\exp\left\{-\frac{L}{2\Theta}(I-\bar{I})^2\right\} dI. \tag{54}$$

In the region of stationary fluctuations the quantity $\bar{I}^2 L/\Theta$ (which is of the same order of magnitude as $(\bar{I}/V)^2 L/C$) is small because of the inequality (53). This enables us to expand (54) in a power series in $\bar{I}$. Restricting ourselves to the first term we have

$$\varphi(\bar{I}) = \beta\bar{I} = R_{eq}\bar{I},$$

where

$$R_{eq} = \frac{1}{\sqrt{2\pi}}\left(\frac{L}{\Theta}\right)^{1/2}\int_{-\infty}^{\infty} V(I)\, I \exp\left\{-\frac{L}{2\Theta}I^2\right\} dI \tag{55}$$

is the equivalent linear resistance by which we can replace the given nonlinear resistance.

The consideration given here was restricted by the condition of fast relaxation of the velocity: $\tau_2 \ll \tau_3$. It would be of great interest to get rid of this restriction.

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APPENDIX

We shall find the coefficients β_{mn} of the expansion (27). We multiply both sides of this equation by $E = \exp[(q-\bar{q})x + (v-\bar{v})y]$ and integrate over q and v. The integral $\int(v-\bar{v})E\tilde{w}\,dq\,dv$ can be written in the form $\partial\Theta(x, y)/\partial y$, where

$$\Theta(x, y) = \int E\tilde{w}\, dq\, dv$$

is the two-dimensional characteristic function of the quantities $q-\bar{q}$ and $v-\bar{v}$. Further integrations by parts give

$$\int\left(-\frac{\partial}{\partial q}\right)^m\left(-\frac{\partial}{\partial v}\right)^n(\beta_{mn}\tilde{w})\, E\, dq\, dv = x^m y^n \beta_{mn}\Theta(x, y).$$

(27) is thus equivalent to the equation

$$\frac{\partial\Theta}{\partial y} = \Theta\Sigma\frac{x^m y^n}{m!n!}\beta_{mn} \quad \text{or} \quad \frac{\partial \ln\Theta}{\partial y} = \Sigma\frac{x^m y^n}{m!n!}\beta_{mn}.$$

At the same time, the two-dimensional characteristic function can, as is well known, be expressed in terms of the cumulants k_{mn} corresponding to the random functions $q-\bar{q}$, $v-\bar{v}$ by the equation

$$\ln\Theta(x, y) = \sum_{m,\,n=1}^{\infty}\frac{x^m y^n}{m!n!}k_{mn}.$$

Equating the last two equations we find

$$\beta_{mn} = k_{mn+1}.$$

If we know the $(m+p)$th velocity correlation function

$$k_{(m+p)v}(t_1, \ldots, t_{m+p}),$$

we can, by integrating, obtain the cumulant

$$k_{mp} = \int_{-\infty}^{t} \cdots \int k_{(m+p)v}(t_1, \ldots, t_m, t, \ldots t)\, dt_1 \ldots dt_m.$$

In particular, we find for the coefficients β_{10} and β_{01} (which are respectively equal to k_{11}, k_{02}) that they are expressed in terms of $k_2(\tau) = k_{(2)v}(t, t+\tau)$ by Eqs. (28).

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160